A Variational Principle for Dissipative Fluid Dynamics

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In the variational principle leading to the Euler equation for a perfect fluid, we can use the method of undetermined multiplier for holonomic constraints representing mass conservation and adiabatic condition. For a dissipative fluid, the latter condition is replaced by the constraint specifying how to dissipate. Noting that this constraint is nonholonomic, we can derive the balance equation of momentum for viscous and viscoelastic fluids by using a single variational principle. We can also derive the associated Hamiltonian formulation by regarding the velocity field as the input in the framework of control theory.

§1. Introduction

In many areas of physics, variational principles help us choose convenient variables in formulating problems. The least-action principle can lead to the equations of motion not only for microscopic dynamics but also those for nondissipative macroscopic dynamics. For example, in a perfect fluid, the sum of the kinetic energy and internal energy is conserved, and we can write down the action easily. There are also the conservation laws for mass and entropy; these holonomic constraints can be incorporated into the action by means of the method of undetermined multipliers. Thus, the Euler equation can be derived from the stationary condition of the action. 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 9

The Navier-Stokes equation is the equation of motion for the Newtonian viscous fluid, and represents the momentum balance with the dissipative force taken into account in the linear phenomenological law.^{10),11)} Without this force, the equation is reduced to the Euler equation. The dissipative force can be derived using another variational principle called the maximum dissipation principle, where Rayleigh's dissipation function is minimized.^{12),13)} Using this principle amounts to assuming the linear phenomenological law. A set of variables with respect to which Rayleigh's dissipation function is minimized is usually different from a set of variables with respect to which the action is stationary.^{14),15)}

One way of unifying these two variational principles is called Onsager's variational principle, $^{16)}$ which has been used frequently in formulating dissipative dynamics of complex fluids. $^{17),18),19),20),21)$ Using this principle, we can obtain the balance equation of momentum with the dissipative force taken into account in the linear phenomenological law. However, applying this principle to the Newtonian fluid in a straightforward way, we can obtain only a linearized version of Navier-Stokes equation, i.e., the Stokes equation. $^{22)}$

A viscous fluid is not locally adiabatic, and the entropy conservation law cannot

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be assumed. We instead impose a constraint specifying how to dissipate. Noting that this constraint is nonholonomic, unlike in the previous studies, we can derive the balance equation of momentum in the framework of a single variational principle. As mentioned above, this framework for a viscous fluid originates from that for a perfect fluid, which we briefly review in §2. Our main results are shown in §3, where we apply our procedure to viscous and viscoelastic fluids. In §4, for completeness, we derive the associated Hamiltonian formulation in the framework of the control theory. Our study is discussed and summarized in the last section.

§2. Perfect fluid

We briefly review Ref. 5) with slight modifications. Let us consider the dynamics of a perfect fluid in a fixed container from the initial time $t_{\rm init}$ to the final time $t_{\rm fin}$. Let V denote the region occupied by the fluid. The velocity field v satisfies nopenetration condition at the boundary ∂V , i.e.,

$$\boldsymbol{n} \cdot \boldsymbol{v} = 0 \text{ on } \partial V ,$$
 (2.1)

where n is the unit normal vector directed outside on ∂V . Let us write ρ for mass per unit volume, and s for entropy per unit mass. The internal-energy density per unit mass, ϵ , is a function of ρ and s because of the local equilibrium. The action is given by the integral of the Lagrangian density with respect to the time and space considered. Apart from the constraints mentioned below, the Lagrangian density is given by

$$\mathcal{L}(\rho, \mathbf{v}, s) \equiv \rho \left\{ \frac{1}{2} \mathbf{v}^2 - \epsilon(\rho, s) \right\} , \qquad (2.2)$$

which is the difference between kinetic energy density and internal energy density. The variables are not independent because of the constraints mentioned below. Writing T and p for the temperature and the pressure, respectively, we have $d\epsilon = -pd\rho^{-1} + Tds$ in the thermodynamics, which leads to

$$p \equiv \rho^2 \left(\frac{\partial \epsilon}{\partial \rho}\right)_s$$
 and $T \equiv \left(\frac{\partial \epsilon}{\partial s}\right)_o$, (2.3)

where the subscripts s and ρ indicate variables fixed in the respective partial differentiations. We write τ for the time in the Lagrangian coordinates although it is equivalent to the time t in the non-relativistic theory. The partial derivatives with respect to τ (∂_{τ}) and t (∂_{t}) imply the Lagrangian and Eulerian time-derivatives, respectively.

In the Lagrangian description, we label a fluid particle with its initial position $\mathbf{a} = (a_1, a_2, a_3)$, and write $\mathbf{X} = (X_1, X_2, X_3)$ for its position at time τ . The time derivative of \mathbf{X} denotes the velocity fields \mathbf{v} , i.e.,

$$\partial_{\tau} X = v . (2.4)$$

The endpoints of the path line are fixed by

$$\delta \mathbf{X}(\mathbf{a}, t_{\text{init}}) = \delta \mathbf{X}(\mathbf{a}, t_{\text{fin}}) = \mathbf{0} .$$
 (2.5)

The volume element in the Lagrangian coordinates can be given by the determinant of the Jacobian matrix,

$$J(\boldsymbol{a},\tau) \equiv \frac{\partial(X_1, X_2, X_3)}{\partial(a_1, a_2, a_3)} \ . \tag{2.6}$$

We assume that J has no singular points in the space and time considered and that $J(\boldsymbol{a}, t_{\text{init}})$ is unity. The conservation law of mass is given by

$$\rho(\boldsymbol{a}, \tau) J(\boldsymbol{a}, \tau) - \rho_{\text{init}}(\boldsymbol{a}) = 0 , \qquad (2.7)$$

where $\rho_{\text{init}}(\boldsymbol{a})$ is the initial value of mass density. The adiabatic condition implies that the entropy of a fluid particle in the perfect fluid is conserved along a path line,

$$s(\boldsymbol{a},\tau) - s_{\text{init}}(\boldsymbol{a}) = 0 , \qquad (2.8)$$

where $s_{\text{init}}(\boldsymbol{a})$ is the initial value of entropy density per mass. Equations (2·7) and (2·8) give holonomic constraints. Using undetermined multipliers, $\boldsymbol{\gamma}$, K and Λ , we can define the action as

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} \int_{V} d^{3}\boldsymbol{a} \left\{ J\mathcal{L}(\rho, s, \boldsymbol{v}) + \boldsymbol{\gamma} \cdot (\partial_{\tau}\boldsymbol{X} - \boldsymbol{v}) + K(\rho J - \rho_{\text{init}}) + \Lambda J(s - s_{\text{init}}) \right\} , \quad (2 \cdot 9)$$

which is a functional of γ , K, Λ , ρ , s, v and X. Taking the variations of Eq. (2.9) with respect to these trajectories, respectively, leads to Eqs. (2.4), (2.7), (2.8),

$$K = -\frac{1}{2}\mathbf{v}^2 + \epsilon + \frac{p}{\rho} \,, \tag{2.10}$$

$$\Lambda = \rho T \tag{2.11}$$

$$\gamma = \rho J \mathbf{v} \tag{2.12}$$

and

$$\frac{\partial}{\partial \tau} \gamma_i = -\frac{\partial}{\partial a_i} \left\{ \rho \left(\frac{1}{2} \boldsymbol{v}^2 - \epsilon + K \right) \frac{\partial J}{\partial (\partial X_i / \partial a_i)} \right\} . \tag{2.13}$$

Roman indices run from 1 to 3, and repeated indices are summed up. The surface integral terms, appearing on the way of this calculation, vanish because of the boundary conditions, Eqs. $(2\cdot1)$ and $(2\cdot5)$. Calculating by means of the cofactors yields

$$\frac{\partial J}{\partial(\partial X_i/\partial a_i)} = J \frac{\partial a_j}{\partial X_i} , \qquad (2.14)$$

while some algebra yields

$$\frac{\partial}{\partial a_j} \left(J \frac{\partial a_j}{\partial X_1} \right) = 0 \ . \tag{2.15}$$

Thus, we can rewrite Eq. (2.13) as

$$\frac{\partial}{\partial \tau} \gamma_i = -J \frac{\partial}{\partial X_i} \left\{ \rho \left(\frac{1}{2} v^2 - \epsilon + K \right) \right\} . \tag{2.16}$$

Substituting Eqs. (2·10) and (2·12) into Eq. (2·16), we successfully obtain the Euler equation in the Lagrangian description,

$$\rho \frac{\partial v_i}{\partial \tau} = -\frac{\partial p}{\partial X_i} \ . \tag{2.17}$$

We can replace $\partial v_i/\partial \tau$ by $(\partial t + \mathbf{v} \cdot \nabla)v_i$ to obtain the Euler equation in the Eulerian description, which is given by Eq. (2·29) below.^{3),4)}

In the Eulerian description, a fluid particle is labeled by the Lagrangian coordinates $\mathbf{A} \equiv (A_1, A_2, A_3)$, which depend on the spatial position \mathbf{x} . Since the Lagrangian coordinates are conserved along the path line, we have

$$\frac{\partial}{\partial t} A_i = -\boldsymbol{v} \cdot \nabla A_i \ . \tag{2.18}$$

The endpoints of a path line are fixed by

$$\delta \mathbf{A}(\mathbf{x}, t_{\text{init}}) = \delta \mathbf{A}(\mathbf{x}, t_{\text{fin}}) = \mathbf{0} , \qquad (2.19)$$

instead of Eq. (2.5), as discussed in Ref. 5). The mass conservation law Eq. (2.7) can be rewritten as

$$\rho(\mathbf{x},t) = J^{-1}(\mathbf{x},t)\rho_{\text{init}}(\mathbf{A}(\mathbf{x},t)) , \qquad (2\cdot20)$$

where the inverse of J is given by

$$J^{-1}(\mathbf{x},t) = \frac{\partial(A_1, A_2, A_3)}{\partial(x_1, x_2, x_3)}.$$
 (2.21)

The action in the Lagrangian description, Eq. (2.9), is rewritten in the Eulerian description as

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} dt \int_{V} d^{3}x \left\{ \mathcal{L}(\rho, s, \boldsymbol{v}) + \beta_{i}(\partial_{t}A_{i} + \boldsymbol{v} \cdot \nabla A_{i}) + K(\rho - \rho_{\text{init}}J^{-1}) + \Lambda(s - s_{\text{init}}) \right\},$$
(2.22)

which is a functional of $\boldsymbol{\beta}$, K, Λ , ρ , s, \boldsymbol{v} and \boldsymbol{A} . The stationary condition of Eq. (2·22) yields Eqs. (2·8), (2·10), (2·11), (2·18), (2·20),

$$\rho \mathbf{v} + \beta_i \nabla A_i = \mathbf{0} \tag{2.23}$$

and

$$\frac{\partial}{\partial t}\beta_i = -\nabla \cdot (\beta_i \mathbf{v}) - KJ^{-1} \frac{\partial \rho_{\text{init}}}{\partial A_i} + \frac{\partial}{\partial x_i} \left\{ K\rho_{\text{init}} \frac{\partial J^{-1}}{\partial (\partial A_i/\partial x_i)} \right\} - \Lambda \frac{\partial s_{\text{init}}}{\partial A_i} \ . \tag{2.24}$$

Here, ρ_{init} and s_{init} depend on \boldsymbol{A} , but ρ and s are independent variables. Using Eqs. (2·8), (2·10), (2·11),

$$\frac{\partial J^{-1}}{\partial (\partial A_i/\partial x_i)} = J^{-1} \frac{\partial x_j}{\partial A_i} \tag{2.25}$$

and

$$\frac{\partial}{\partial x_j} \left(J^{-1} \frac{\partial x_j}{\partial A_i} \right) = 0 , \qquad (2.26)$$

we can rewrite Eq. (2.24) as

$$\frac{\partial}{\partial t}\beta_{i} = -\nabla \cdot (\beta_{i}\boldsymbol{v}) + \left(\rho \frac{\partial K}{\partial x_{j}} - \rho T \frac{\partial s}{\partial x_{j}}\right) \frac{\partial x_{j}}{\partial A_{i}}$$

$$= -\nabla \cdot (\beta_{i}\boldsymbol{v}) + \left(-\frac{\rho}{2} \frac{\partial \boldsymbol{v}^{2}}{\partial x_{j}} + \frac{\partial p}{\partial x_{j}}\right) \frac{\partial x_{j}}{\partial A_{i}}.$$
(2.27)

Dividing Eq. (2.23) by ρ , we calculate the Lie derivative of the resulting equation with respect to \boldsymbol{v} to find the sum of the Lie derivative of \boldsymbol{v} and

$$(\nabla A_i) \left(\frac{\partial}{\partial t} + \boldsymbol{v} \cdot \nabla \right) \left(\frac{\beta_i}{\rho} \right) \tag{2.28}$$

to vanish, with the aid of Eq. (2·18). The Lie derivative of v was given in Appendix A of Ref. 5). Substituting Eq. (2·27) into Eq. (2·28), we can derive the Euler equation,

$$\rho \left\{ \frac{\partial}{\partial t} \boldsymbol{v} + \frac{1}{2} \nabla \boldsymbol{v}^2 - \boldsymbol{v} \times (\nabla \times \boldsymbol{v}) \right\} = -\nabla p . \qquad (2.29)$$

§3. Dissipative fluids

3.1. Simple dissipative system

To show the essence of our procedure, we consider a damped harmonic oscillator in a heat bath. We define the position of the oscillator, q, so that it vanishes in the balance. We write m and k for the mass of the oscillator and the spring constant, respectively. The internal energy of the heat bath, E, is a function of its entropy, S, and its temperature is given by $T \equiv dE/dS$. We assume that the frictional force, f, is exerted on the oscillator. The action is given by the integral of the difference between the kinetic energy and the sum of the potential energy and the internal energy over the time interval $[t_{\rm init}, t_{\rm fin}]$,

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} dt \left\{ \frac{1}{2} m \left(\frac{dq}{dt} \right)^2 - \left(\frac{1}{2} kq^2 + E(S) \right) \right\} , \qquad (3.1)$$

which is a functional of trajectories q(t) and S(t). The frictional force converts the mechanical energy into heat. Thus, the realized trajectories should satisfy

$$f\frac{dq}{dt} + T\frac{dS}{dt} = 0 , (3.2)$$

considering that the heat bath is always at the equilibrium. Any trajectory making the action stationary under the constraint of

$$f\delta q + T\delta S = 0 \tag{3.3}$$

satisfies Eq. (3.2) because the infinitesimal variations δS and δq can be those in the direction of the time. Change in the entropy generally should depend on how the oscillator is moved in the time interval from $t_{\rm init}$ to $t_{\rm fin}$, in terms of the thermodynamics. Thus, for example, the constraint of $\delta q = 0$ at $t_{\rm fin}$ in the variational

calculation does not always mean that of $\delta S = 0$ at $t_{\rm fin}$. Hence, then the constraint Eq. (3·3) is generally nonholonomic because it cannot be rewritten in a form that the infinitesimal variation of a function, U, of q and S always vanishes, i.e., $\delta U = 0$. (12)

The variation of the action Eq. (3.1) yields

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} dt \left\{ \left(-m \frac{d^2 q}{dt^2} - kq \right) \delta q - T \delta S \right\} = 0 . \tag{3.4}$$

Here, we fix both ends of the trajectory of q, i.e.,

$$\delta q(t_{\rm init}) = \delta q(t_{\rm fin}) = 0 . \tag{3.5}$$

Substituting Eq. (3·3) into Eq. (3·4) gives the balance equation of momentum,

$$m\frac{d^2q}{dt^2} = -kq + f \ . \tag{3.6}$$

The frictional force, f, is given by $-\xi dq/dt$ with ξ being the friction coefficient, according to the linear phenomenological law. This simple model can be regarded as a simple Kelvin-Voigt model of the viscoelasticity. If the damping follows the Maxwell model, the second term on the left-hand side (lhs) of Eq. (3·2) should be replaced by the frictional force multiplied by the deformation rate of the viscous part (dash-pot). This model is discussed in §3.3.

Let us consider whether a straightforward way of applying the method of undetermined multipliers to the constraint Eq. (3.2) works well. Modifying the action so that it contains the product of the multiplier and the lhs of Eq. (3.2), we encounter

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} dt \left\{ \xi \frac{d^2 q}{dt^2} \delta q + \left(\frac{dT}{dS} - \frac{dT}{dt} \right) \delta S \right\} + \left[-\frac{d^2 q}{dt^2} \delta q \right]_{t_{\text{init}}}^{t_{\text{fin}}} + [T \delta S]_{t_{\text{init}}}^{t_{\text{fin}}} = 0 , \qquad (3.7)$$

where we assumed that T is a function of S, in calculating the stationary condition of the modified action. Because the last term on the lhs of Eq. (3.7) does not always vanish under Eq. (3.5), it is found that we cannot derive Eq. (3.6) in this way.

3.2. Viscous fluid

For a viscous fluid, we write σ_{ij} and J_q for the viscous stress tensor and the heat flux, respectively. Let us define the rate-of-strain tensor e_{ij} as $(\partial_j v_i + \partial_i v_j)/2$, and the equation corresponding to Eq. (3·2) turns out to be

$$\rho T \left(\partial_t + \boldsymbol{v} \cdot \nabla \right) s - \sigma_{ij} e_{ij} + \nabla \cdot \boldsymbol{J}_q = 0 \ . \tag{3.8}$$

We assume the no-slip boundary condition

$$\mathbf{v} = \mathbf{0} \quad \text{on} \quad \partial V \,, \tag{3.9}$$

instead of Eq. (2·1), and thus, we can assume no dissipation at the boundary. We assume that the whole fluid is enclosed by an adiabatic wall, i.e., that no heat flux cannot pass through the boundary. It enables us to integrate Eq. (3·8) over V to obtain

$$\int_{V} d^{3} \boldsymbol{a} \left\{ J \left(\rho T \frac{\partial s}{\partial \tau} + \boldsymbol{f} \cdot \frac{\partial \boldsymbol{X}}{\partial \tau} \right) \right\} = 0 . \tag{3.10}$$

Here, $\boldsymbol{f} = \nabla \cdot \boldsymbol{\sigma}^T$ is the dissipative force per unit volume, with the superscript T indicating the transposition. In the Lagrangian description, as in Eq. (3·3), we thus impose the nonholonomic constraint,

$$\int_{V} d^{3}\boldsymbol{a} \left\{ J\left(\rho T \delta s + \boldsymbol{f} \cdot \delta \boldsymbol{X}\right) \right\} = 0 , \qquad (3.11)$$

instead of the adiabatic condition Eq. (2.8) for the perfect fluid. Thus, the action, Eq. (2.9), for the perfect fluid can be rewritten into the action for the viscous fluid as

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} d\tau \int_{V} d^{3}\boldsymbol{a} \left\{ J\mathcal{L}(\rho, s, \boldsymbol{v}) + \boldsymbol{\gamma} \cdot (\partial_{\tau}\boldsymbol{X} - \boldsymbol{v}) + K(\rho J - \rho_{\text{init}}) \right\} , \qquad (3.12)$$

which is a functional of γ , K, ρ , s, v and X. The stationary condition of this action under the constraint, Eq. (3·11), can be obtained, as Eq. (3·6) is derived from Eqs. (3·1) and (3·3). Thus, we obtain Eqs. (2·4), (2·7), (2·10), (2·12) and

$$\frac{\partial \gamma_i}{\partial \tau} = -\frac{\partial}{\partial a_j} \left\{ \rho \left(\frac{1}{2} v^2 - \epsilon + K \right) \right\} \frac{\partial J}{\partial (\partial X_i / \partial a_j)} + J f_i . \tag{3.13}$$

Substituting Eqs. $(2\cdot10)$ and $(2\cdot12)$ into Eq. $(3\cdot13)$, we successfully obtain the balance equation of momentum for the viscous fluid in the Lagrangian description,

$$\rho \frac{\partial v_i}{\partial \tau} = -\frac{\partial p}{\partial X_i} + f_i . \tag{3.14}$$

As in $\S 2$, we can formulate the variational principle in the Eulerian description. Let us rewrite Eq. (3.10) as

$$\int_{\mathbf{V}} d^3 \mathbf{x} \left\{ \rho T \left(\partial_t s + \mathbf{v} \cdot \nabla s \right) + \mathbf{f} \cdot \mathbf{v} \right\} = 0 . \tag{3.15}$$

From Eq. (2.18), we can derive

$$v_j = -\frac{\partial x_j}{\partial A_i} \frac{\partial A_i}{\partial t} , \qquad (3.16)$$

which can also be derived from differentiating x(A(x,t),t) = x with respect to t. By means of Eq. (3·16), the nonholonomic constraint Eq. (3·11) can be rewritten as

$$\int_{\mathbf{V}} d^3 \mathbf{x} \left\{ \rho T \delta s - \frac{\partial x_j}{\partial A_i} \left(\rho T \frac{\partial s}{\partial x_j} + f_j \right) \delta A_i \right\} = 0 . \tag{3.17}$$

The action, Eq. $(2\cdot22)$, can be rewritten as

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} dt \int_{V} d^{3}x \left\{ \mathcal{L}(\rho, s, \boldsymbol{v}) + \beta_{i} (\partial_{t} A_{i} + \boldsymbol{v} \cdot \nabla A_{i}) + K(\rho - \rho_{\text{init}} J^{-1}) \right\} , \qquad (3.18)$$

which is a functional of β , K, ρ , s, v and A. Calculating the stationary condition of this action under the nonholonomic constraint, Eq. (3·17), we can obtain Eqs. (2·10),

(2.18), (2.20), (2.23) and

$$\frac{\partial}{\partial t}\beta_{i} = -\nabla \cdot (\beta_{i}\boldsymbol{v}) + \left(\rho \frac{\partial K}{\partial x_{j}} - \rho T \frac{\partial s}{\partial x_{j}} - f_{j}\right) \frac{\partial x_{j}}{\partial A_{i}}$$

$$= -\nabla \cdot (\beta_{i}\boldsymbol{v}) + \left(-\rho \frac{1}{2} \frac{\partial \boldsymbol{v}^{2}}{\partial x_{j}} + \frac{\partial p}{\partial x_{j}} - f_{j}\right) \frac{\partial x_{j}}{\partial A_{i}}.$$
(3.19)

Following the same procedure as shown just below Eq. (2.27), we find that Eqs. (2.18), (2.23) and (3.19) yield

$$\rho \left\{ \frac{\partial}{\partial t} \boldsymbol{v} + \frac{1}{2} \nabla \boldsymbol{v}^2 - \boldsymbol{v} \times (\nabla \times \boldsymbol{v}) \right\} = -\nabla p + \nabla \cdot \sigma^T , \qquad (3.20)$$

which is equivalent to Eq. (3·14). The viscous stress tensor σ_{ij} is a symmetric tensor because the angular momentum is conserved, as shown in Appendix A. If the viscous stress tensor σ is given in the linear phenomenological law, each of Eqs. (3·14) and (3·20) represents the Navier-Stokes equation.

3.3. Viscoelastic fluid

We consider a viscoelastic fluid. We still write e_{ij} for the rate-of-strain tensor of the fluid, while we write E_{ij} for the strain tensor of the elastic part and $\check{\sigma}_{ij}$ for the viscous stress tensor of the viscous part. The internal energy, ϵ_e , is a function of ρ , s and E_{ij} , and satisfies

$$d\epsilon_e = -pd\rho^{-1} + Tds + \rho^{-1}\kappa_{ij}dE_{ij} , \qquad (3.21)$$

whereby κ_{ij} is defined. We assume the rate-of-strain tensor of the viscous part to be given by

$$\check{e}_{ij} \equiv e_{ij} - (\partial_t + \boldsymbol{v} \cdot \nabla) E_{ij} . \tag{3.22}$$

We can assume that Eq. (3.8) holds if the second term on its lhs is replaced by $-\check{\sigma}_{ij}\check{e}_{ij}$. In the Eulerian description, the resultant equation is

$$\int_{\mathbf{V}} d^3 \mathbf{x} \left\{ \rho T \left(\partial_t s + \mathbf{v} \cdot \nabla s \right) + \left(\partial_k \check{\sigma}_{jk} + \check{\sigma}_{kl} \partial_j E_{kl} \right) v_j + \check{\sigma}_{ij} \partial_t E_{ij} \right\} = 0 . \tag{3.23}$$

Using the same procedure in §3.2, we have the nonholonomic constraint,

$$\int_{\mathbf{V}} d^3 \mathbf{x} \left\{ \rho T \delta s - \frac{\partial x_j}{\partial A_i} \left(\rho T \frac{\partial s}{\partial x_j} + \frac{\partial \check{\sigma}_{jk}}{\partial x_k} + \check{\sigma}_{kl} \frac{\partial E_{kl}}{\partial x_j} \right) \cdot \delta A_i + \check{\sigma}_{ij} \delta E_{ij} \right\} = 0 . \quad (3.24)$$

The Lagrangian density is given by

$$\mathcal{L}_{e}(\rho, \boldsymbol{v}, s, E_{ij}) \equiv \rho \left\{ \frac{1}{2} \boldsymbol{v}^{2} - \epsilon_{e}(\rho, s, E_{ij}) \right\} . \tag{3.25}$$

Replacing \mathcal{L} in Eq. (3·18) by \mathcal{L}_{e} , we obtain the action, the stationary condition of which with respect to δA_{i} turns out to be

$$\frac{\partial}{\partial t}\beta_{i} = -\nabla \cdot (\beta_{i}\boldsymbol{v}) + \left(\rho \frac{\partial K}{\partial x_{j}} - \rho T \frac{\partial s}{\partial x_{j}} - \frac{\partial \check{\sigma}_{jk}}{\partial x_{k}} - \check{\sigma}_{kl} \frac{\partial E_{kl}}{\partial x_{j}}\right) \frac{\partial x_{j}}{\partial A_{i}}$$

$$= -\nabla \cdot (\beta_{i}\boldsymbol{v}) + \left(-\rho \frac{1}{2} \frac{\partial \boldsymbol{v}^{2}}{\partial x_{j}} + \frac{\partial p}{\partial x_{j}} - \frac{\partial \check{\sigma}_{jk}}{\partial x_{k}}\right) \frac{\partial x_{j}}{\partial A_{i}}, \tag{3.26}$$

with the aid of Eq. (3.24), as Eq. (2.27) is derived. With respect to δE_{ij} , we have

$$\kappa_{ij} = \check{\sigma}_{ij} \ . \tag{3.27}$$

Using the same procedure in §3.2, we have the balance equation of the momentum in the Eulerian description, which equals Eq. (3·20) with σ_{ij} replaced by $\check{\sigma}_{ij}$. Calculations in the Lagrangian description can also be performed as in §3.2.

Within the linear phenomenological law, assuming $\check{\sigma}_{ij}$ to be linear with respect to \check{e}_{ij} and κ_{ij} with respect to E_{ij} , we can find

$$(\partial_t + \boldsymbol{v} \cdot \nabla) \check{\sigma}_{ij} \tag{3.28}$$

to be linear with respect to $e_{ij} - \check{e}_{ij}$. Here, \check{e}_{ij} is linear with respect to $\kappa_{ij} = \check{\sigma}_{ij}$. This gives the viscoelasticity of the Maxwell type.^{23),24)}

Equation (3·22) represents how the strain tensor is convected. Under mathematical notation, the last term on the right-hand side (rhs) of Eq. (3·21) should be $\rho^{-1}\kappa_i^j dE_j^i$, for example. If \check{e}_{ij} , e_{ij} and E_{ij} are respectively replaced by \check{e}_j^i , e_j^i and E_j^i in Eq. (3·22), the way of convection of the contravariant tensor E^{ij} involves the upper convected time derivative. Hence, then what we have considered here is the viscoelasticity of the upper convected Maxwell type within the linear phenomenological law.¹⁸)

3.4. Two-component fluid

We consider a two-component fluid. Let ρ_a and ρ_b be the mass densities of components a and b, respectively. The total mass density is given by $\rho \equiv \rho_a + \rho_b$, and the mass fraction of component a is $\psi \equiv \rho_a/\rho$. We define the chemical potential as the Gibbs energy per unit mass, and write μ for the difference given by subtracting the chemical potential of the component b from that of a. The internal energy per mass is a function of ρ_a , ρ_b and s, for which we write $\epsilon_2(\rho_a, \rho_b, s)$. We have

$$d\epsilon_2 = \frac{p}{\rho^2} d\rho + \mu d\psi + T ds , \qquad (3.29)$$

which can be rewritten in terms of $d\rho_a$, $d\rho_b$ and ds with the aid of

$$d\rho = d\rho_a + d\rho_b \tag{3.30}$$

and

$$d\psi = \frac{1 - \psi}{\rho} d\rho_a - \frac{\psi}{\rho} d\rho_b \ . \tag{3.31}$$

The components a and b have their respective velocities \mathbf{v}_a and \mathbf{v}_b and Lagrangian coordinates \mathbf{A}_a and \mathbf{A}_b . The mean velocity of the fluid is given by $\mathbf{v} \equiv \psi \mathbf{v}_a + (1 - \psi)\mathbf{v}_b$. The equations corresponding to Eqs. (2·21) and (3·16) can be respectively written as

$$J_c^{-1} = \frac{\partial (A_{c1}, A_{c2}, A_{c3})}{\partial (x_1, x_2, x_3)} , \qquad (3.32)$$

and

$$v_{cj} = -\frac{\partial x_{cj}}{\partial A_{ci}} \frac{\partial A_{ci}}{\partial t} , \qquad (3.33)$$

where c = a, b. The Lagrangian density is given by

$$\mathcal{L}_2(\rho_a, \rho_b, s, \boldsymbol{v}_a, \boldsymbol{v}_b) \equiv \frac{1}{2}\rho \boldsymbol{v}^2 - \rho \epsilon_2(\rho_a, \rho_b, s) . \tag{3.34}$$

In general, the dissipation is associated with the fluid viscosity, the heat conduction and the mutual diffusion. Here, we consider a polymer solution, where the components a and b are a polymer and a solvent, respectively. For simplicity, we neglect the polymer elasticity and fluid viscosity, although they can be considered as in the preceding subsections. We have

$$\rho T \left(\partial_t + \boldsymbol{v} \cdot \nabla \right) s + \boldsymbol{\xi} \cdot (\boldsymbol{v}_a - \boldsymbol{v}_b) + \nabla \cdot \boldsymbol{J}_{\boldsymbol{q}} = 0 , \qquad (3.35)$$

where ξ denotes the frictional force. As we derive Eq. (3.17), we can obtain

$$\int_{\mathbf{V}} d^3 \mathbf{x} \left\{ \rho T \delta s - \sum_{c=a,b} \frac{\partial x_{cj}}{\partial A_{ci}} \left(\rho_c T \frac{\partial s}{\partial x_j} + \xi_{cj} \right) \delta A_{ci} \right\} = 0 , \qquad (3.36)$$

where $\boldsymbol{\xi}_a$ and $\boldsymbol{\xi}_b$ are introduced to satisfy $\boldsymbol{\xi}_a = -\boldsymbol{\xi}_b = \boldsymbol{\xi}$. As in §3.2, the action is a functional of $\boldsymbol{\beta}_c$, K_c , ρ_c , s, \boldsymbol{v}_c and \boldsymbol{A}_c with c running from a to b, and given by

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} dt \int_{V} d^{3}\boldsymbol{x} \left[\mathcal{L}_{2} + \sum_{c=a,b} \left\{ \beta_{ci} (\partial_{t} A_{ci} + \boldsymbol{v}_{c} \cdot \nabla A_{ci} + K_{c} (\rho_{c} - \rho_{c \text{ init}} J_{c}^{-1}) \right\} \right] , \quad (3.37)$$

where $\rho_{c \text{ init}}$ is the initial mass density of the component c. Under the nonholonomic constraint Eq. (3·36), we find the stationary condition of Eq. (3·37) to be

$$\rho_c - \rho_{c \text{ init}} J_c^{-1} = 0 , \qquad (3.38)$$

$$\rho_c \mathbf{v} + \beta_{ci} \nabla A_{ci} = \mathbf{0} , \qquad (3.39)$$

$$\frac{\partial}{\partial t}\beta_{ci} = -\nabla \cdot (\beta_{ci}\boldsymbol{v}_c) + \left(\rho_c \frac{\partial K_c}{\partial x_j} - \rho_c T \frac{\partial s}{\partial x_j} - \xi_{cj}\right) \frac{\partial x_{cj}}{\partial A_{ci}}$$
(3.40)

and

$$K_c = \left(\frac{1}{2}\boldsymbol{v}^2 - \boldsymbol{v}_c \cdot \boldsymbol{v}\right) + \epsilon + \frac{p}{\rho} + \mu_c \left(1 - \frac{\rho_c}{\rho}\right) , \qquad (3.41)$$

where μ_a and μ_b are introduced to satisfy $\mu_a = -\mu_b = \mu$. As in §3.2, we can derive the balance equations of momentum for the components,

$$\rho_c \left\{ \frac{\partial}{\partial t} \boldsymbol{v} + \frac{1}{2} \nabla \boldsymbol{v}^2 - \boldsymbol{v}_c \times (\nabla \times \boldsymbol{v}) \right\} = -\frac{\rho_c}{\rho} \nabla p + \frac{\rho_a \rho_b}{\rho} \nabla \mu_c + \boldsymbol{\xi}_c . \tag{3.42}$$

The sum of Eq. (3·42) over c=a,b gives Eq. (3·20) with $\nabla \cdot \sigma^T$ deleted. The resultant equation describes the momentum balance of the solution as a whole. The calculations in this subsection are in the Eulerian description; those in the Lagrangian description can be performed as in §3.2.

§4. Hamiltonian formulation

Applying the control theory^{25), 26)} to the dynamics of the perfect fluid, we derived its Hamiltonian formulation.⁵⁾ Similarly, with slight modifications as shown below, we can derive the Hamiltonian formulation for dissipative dynamics. In the control theory, a subsystem controlled by another subsystem is called a plant. Let q and u denote the plant state and the input to the plant, respectively. We assume that the plant dynamics follows

$$\frac{d}{dt}q(t) - F(q(t), u(t)) = 0 , \qquad (4.1)$$

whereby a function F is defined. In addition to q and u, we assume that the Lagrangian, L, also depends on a variable S, which will denote the entropy in the later application to dissipative dynamics. In the control theory, we define an evaluation functional

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} dt \ L(q, u, S) \ , \tag{4.2}$$

and determine the optimal input u^* so that the evaluation functional is minimized under the constraint given by Eq. (4·1). We also require Eq. (3·3) and $T \equiv -\partial L/\partial S$.

We take the constraints into account using the undetermined multiplier, p, which is called costate in the control theory. The functional to be minimized, which we call action, can be defined as

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} dt \left\{ L(q, u, S) + p \left(\frac{dq}{dt} - F(q, u) \right) \right\} . \tag{4.3}$$

Let $u^{\sharp}(q, p, S)$ denote the input minimizing Eq. (4·3) on condition that q, p and S are fixed. This means that the time integral of $\tilde{H} \equiv -L(q, u, S) + pF(q, u)$ from t_{init} to t_{fin} is stationary with respect to u at $u = u^{\sharp}(q, p, S)$. Let us define

$$H(q, p, S) \equiv \tilde{H}(q, u^{\sharp}(q, p, S), p, S) , \qquad (4.4)$$

which is usually called the Hamiltonian. The preoptimized action is defined as

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} dt \left\{ -H(q, p, S) + p \frac{d}{dt} q \right\} , \qquad (4.5)$$

which is a functional of q, S and p. The optimal input u^* is given by $u^{\sharp}(q, p, S)$, when q, p and S satisfy the stationary condition of Eq. (4·5) under Eqs. (3·3) and (3·5). We can usually assume $\partial^2 L/(\partial S \partial u)$ to vanish, and thus u^{\sharp} is a function of only q and p. In this case, we find

$$\frac{\partial H}{\partial S} = -\frac{\partial L}{\partial S} = T \ . \tag{4.6}$$

Using Eqs. (3·3), (3·5), (4·5) and (4·6), we obtain a set of modified Hamilton's equations, which are Eq. (3·2),

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} \tag{4.7}$$

and

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q} + f \ . \tag{4.8}$$

In a straightforward way from Eqs. (3·2), (4·7) and (4·8), we have dH/dt=0. Further discussion is given in Appendix A.

Let us apply the formulation above to the viscous fluid discussed in §3.2. In the Eulerian description, the state, costate, entropy density and input are respectively given by $\mathbf{A}, \boldsymbol{\beta}, s$ and \mathbf{v} . Equation (4·1) is given by (2·18) in this fluid, where the function corresponding to \tilde{H} is given by

$$\tilde{\mathcal{H}}(\boldsymbol{A}, \boldsymbol{v}, \boldsymbol{\beta}, s) \equiv -\rho \left\{ \frac{1}{2} \boldsymbol{v}^2 - \epsilon(\rho, s) \right\} + \beta_i \boldsymbol{v} \cdot \nabla A_i . \tag{4.9}$$

Here, ρ is regarded as a function of \boldsymbol{A} given by Eq. (2·20) without the undetermined multiplier K introduced. Let $\boldsymbol{v}^{\sharp}(\boldsymbol{A},\boldsymbol{\beta})$ denote the input corresponding to u^{\sharp} , and we find the Hamiltonian to be given by the sum of the kinetic and inertial-energy densities,

$$\mathcal{H}(\mathbf{A}, \boldsymbol{\beta}, s) \equiv \rho \left\{ \frac{1}{2} \mathbf{v}^{\sharp 2} + \epsilon(\rho, s) \right\} , \qquad (4.10)$$

where v^{\sharp} satisfies Eq. (2·23). The modified Hamilton's equations can be found to be Eqs. (2·18) and (3·19). In deriving these equations, we note that, for example,

$$\frac{\delta}{\delta\beta_i} = \frac{\partial}{\partial\beta_i} - \frac{\partial}{\partial x_i} \frac{\partial}{\partial(\partial_i\beta_i)} \tag{4.11}$$

should replace $\partial/\partial p$ in Eq. (4·7) because the fields are involved here unlike in Eqs. (4·7) and (4·8). In the Lagrangian description, v^{\sharp} satisfies Eq. (2·12), and the modified Hamilton's equations are found to be Eqs. (2·4) and (2·16) with v replaced by v^{\sharp} .

§5. Discussion

It is natural that the nondissipative equation can be derived by means of the least-action principle. We can formulate dissipative dynamics by adding the dissipative force to the equation of motion to this nondissipative equation. In this formulation, the variational principle is inherent to the nondissipative dynamics. We can obtain the dissipative force by means of the maximum dissipation principle, where the linear phenomenological law is simply derived from the stationary condition of the quadratic form. These two variational principles have been utilized especially in formulating dynamics of complex fluids, as mentioned in §1.

In the irreversible thermodynamics for a one-component viscous fluid, ^{10), 11)} we start with the mass conservation law, the balance equations of momentum and energy. Then, combining these equations with the local equilibrium yields Eq. (3·8) from which the rate of the total entropy production is written in terms of fluxes and thermodynamic forces.²⁷⁾ The linearity between them is assumed to give the linear phenomenological law, determining the dissipative force near the equilibrium.

Suppose that we do not know the balance equation of momentum but know Eq. (3.8), representing how the dissipation occurs. Still, we can calculate the rate of the total entropy production from Eq. (3.8), and then we can determine the dissipative force within the linear phenomenological law. On the other hand, we can derive the balance equation of momentum from Eq. (3.8) by retracing a part of the calculations mentioned in the preceding paragraph. What we do in this work is to formulate this derivation in a single variational principle.

This variational principle is easy to understand in terms of physics. The least-action principle for the perfect fluid is associated with the entropy conservation law. Replacing this constraint on the entropy with a constraint describing how the dissipation changes the entropy, we can obtain our variational principle. The key point inherent to the dissipative dynamics is to appreciate that this is the nonholonomic constraint to which the method of undetermined multipliers cannot be applied.

Applications of this variational principle to a viscous fluid, a viscoelastic fluid and a two-component fluid are shown in §3. They are straightforward generalizations of the simple case discussed in §3.1. We believe that this principle can be easily applied to the dynamics of other complex fluids, such as liquid crystals and electromagnetic fluids.^{20),21)}

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We show that the Hamiltonian version of Noether's theorem^{12),28)} still works for the model discussed in §4. Let us consider a canonical transformation, mapping (q_0, p_0, S_0) to $(q_\alpha, p_\alpha, S_\alpha)$, which makes the modified Hamilton's equations, Eqs. (3·2), (4·7) and (4·8), invariant. When the transformation with respect to α is infinitesimal, the generator $G(q_0, p_\alpha, S_0, t)$ can be defined. Then, because of the canonical transformation, we have

$$\int_{t_{\text{init}}}^{t_{\text{fin}}} dt \left\{ p_0 \dot{q}_0 - H_0(q_0, p_0, S_0) \right\} = \int_{t_{\text{init}}}^{t_{\text{fin}}} dt \left\{ p_\alpha \dot{q}_\alpha - H_\alpha(q_\alpha, p_\alpha, S_\alpha) + \frac{d}{dt} \left(q_0 p_\alpha + \alpha G \right) \right\}, \tag{A.1}$$

where (q_0, p_0, S_0) and $(q_\alpha, p_\alpha, S_\alpha)$ respectively satisfy the modified Hamilton's equations. With the aid of Eqs. (3·2) and (3·5), Eq. (A·1) yields

$$\delta q \equiv q_{\alpha} - q_0 = \alpha \frac{\partial G}{\partial p_0} , \qquad (A.2)$$

$$\delta p \equiv p_{\alpha} - p_0 = \alpha \left(-\frac{\partial G}{\partial q_0} + \frac{f}{T} \frac{\partial G}{\partial S_0} \right)$$
 (A·3)

and

$$H_{\alpha}(q_{\alpha}, p_{\alpha}, S_{\alpha}) - H_{0}(q_{0}, p_{0}, S_{0}) = \alpha \frac{\partial G}{\partial t}$$
, (A·4)

where we simply wrote G for $G(q_0, p_0, S_0, t)$. From Eqs. (3·3), (4·6)–(4·8), (A·2) and (A·3), we have

$$H_{\alpha}(q_{\alpha}, p_{\alpha}, S_{\alpha}) = H_{\alpha}(q_{0}, p_{0}, S_{0}) + \frac{\partial H}{\partial q} \delta q + \frac{\partial H}{\partial p} \delta p + \frac{\partial H}{\partial S} \delta S$$
 (A·5)

$$= H_{\alpha}(q_0, p_0, S_0) - \alpha \left(\frac{dp}{dt} \frac{\partial G}{\partial p} + \frac{dq}{dt} \frac{\partial G}{\partial q} + \frac{dS}{dt} \frac{\partial G}{\partial S} \right) . \quad (A.6)$$

Substituting Eq. $(A \cdot 6)$ into Eq. $(A \cdot 4)$ yields

$$H_{\alpha}(q_0, p_0, S_0) - H_0(q_0, p_0, S_0) = \alpha \frac{dG}{dt}$$
 (A·7)

Thus, the condition dG/dt = 0 is equivalent to the invariance of H, i.e., $H_{\alpha} = H_0$, under the canonical transformation. If time-invariant, H is the generator of the infinitesimal canonical transformation with respect to the time.

As discussed in §4, the Hamiltonian density of a fluid is given by $\mathcal{H}(\mathbf{A}, \boldsymbol{\beta}, s)$ of Eq. (4·10), where \mathbf{A} , $\boldsymbol{\beta}$ and s are respectively the state, costate and entropy density. As Eq. (A·7), we can derive

$$\int_{V} d^{3}x \left\{ \mathcal{H}_{\alpha}(\boldsymbol{A}_{0}, \boldsymbol{\beta}_{0}, s_{0}) - \mathcal{H}_{0}(\boldsymbol{A}_{0}, \boldsymbol{\beta}_{0}, s_{0}) \right\} = \int_{V} d^{3}x \, \alpha \frac{d\mathcal{G}}{dt} . \tag{A.8}$$

Thus, if \mathcal{H} is invariant under the transformation generated by \mathcal{G} , the integral of \mathcal{G} over V is conserved. This means that a vector field \mathbf{J} can be defined so that

$$\frac{\partial \mathcal{G}}{\partial t} + \nabla \cdot \boldsymbol{J} = 0 \tag{A.9}$$

is satisfied and that the surface integration of $J \cdot n$ over ∂V vanishes. Its converse also holds. The spatial transformation is generated by the momentum, $\rho v^{\sharp} = -\beta_i \nabla A_i$. The total momentum of the fluid is conserved when there are no external forces acting on the boundary ∂V . It is thus natural that we can rewrite Eq. (3·20) in the form of Eq. (A·9), i.e.,

$$\frac{\partial}{\partial t}(\rho v_i^{\sharp}) + \partial_j(\rho v_i^{\sharp} v_j^{\sharp} - T_{ij}) = 0 , \qquad (A \cdot 10)$$

where $T_{ij} \equiv p\delta_{ij} - \sigma_{ij}$ is a stress tensor. The spatial rotation is generated by the angular momentum, $\mathbf{l} \equiv \rho \mathbf{x} \times \mathbf{v}^{\sharp} = -\mathbf{x} \times \beta_i \nabla A_i$. The total angular momentum of the fluid is conserved when there is no external torque acting on the boundary ∂V . The time evolution of \mathbf{l} turns out to be

$$\frac{\partial l_i}{\partial t} + \frac{\partial}{\partial x_l} \left(l_i v_l^{\sharp} - \epsilon_{ijk} x_j T_{kl} \right) - \epsilon_{ijk} T_{kj} = 0 , \qquad (A.11)$$

with the aid of Eq. (A·10), where the Levi-Civita symbol ϵ_{ijk} is anti-symmetric on each pair of indices. The last term on the lhs above should vanish from the discussion just around Eq. (A·9), which leads to $\sigma_{ij} = \sigma_{ji}$.

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